

A new deformed Schiöberg-type potential and ro-vibrational energies for some diatomic molecules

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We suggest a new deformed Schiöberg-type potential for diatomic molecules. We show that it is equivalent to Tietz-Hua oscillator potential. We discuss how to relate our deformed Schiöberg potential to Morse, to Deng-Fan, to the improved Manning-Rosen, and to the deformed modified Rosen-Morse potential models. We transform our potential into a proper form and use the super-symmetric quantization to find a closed form analytical solution for the ro-vibrational energy levels that are highly accurate over a wide range of vibrational and rotational quantum numbers. We discuss our results using 4-diatomic molecules $\text{NO}(X^2\Pi_r)$, $\text{O}_2(X^3\Sigma_g^-)$, $\text{O}_2^+(X^2\Pi_g)$, and $\text{N}_2(X^1\Sigma_g^+)$. Our results turn out to compare excellently with those from a generalized pseudospectral numerical method.

Keywords: Diatomic molecular potentials, Deformed Schiöberg-type potential Ro-vibrational energies.

I. INTRODUCTION

An empirical diatomic potential energy function provides a quantitative description of the energy-distance relation that encodes within the relevant information about a diatomic molecule. Consequently, a large number of empirical potential models has been suggested [1–10]. Improved, extended and/or deformed forms of these potentials were investigated in the literature [11–28]. For example, an extended Lennard-Jones potential is tested by Hajigeorgiou [13], a deformed and shifted-by-a-constant Rosen-Morse potential [13, 17] is studied and found to be equivalent to the known Tietz [7] and Wei [10] potentials, Wang et al. [12] have shown the equivalence of three potential models (Manning-Rosen [3], Schiöberg [9], and Deng-Fan [5]), an improved Schiöberg potential energy model is studied by Wang et al. [15], etc. Nevertheless, the dependence of the transition probabilities on the rotational-vibrational (ro-vibrational hereinafter) energy levels has inspired the search for closed-form analytical energy expressions that are accurate over a broad range of rotational and vibrational quantum numbers. Such closed-form expressions provide a substantial simplification of the derivations of the transition probabilities and are of great advantage in the studies of molecular transitions in gases, where different collision systems would identify the gas properties [19].

However, the main challenge in finding the ro-vibrational energy levels lies in dealing with the central rotational core, $J(J+1)/2\mu r^2$ with $J \neq 0$, of the radial spherically symmetric Schrödinger equation

$$-\frac{\hbar^2}{2\mu} \frac{d^2 R_{\nu,J}(r)}{dr^2} + \left[\frac{J(J+1)\hbar^2}{2\mu r^2} + U(r) \right] R_{\nu,J}(r) = E_{\nu,J} R_{\nu,J}(r), \quad (1)$$

where ν denotes the vibrational and J denotes the rotational quantum numbers. This equation is known to be exactly solvable in a closed form for $J = 0$. Whereas, for $J \neq 0$ one needs to use an approximation for the central rotational core term and obtain a closed form analytical solution (cf, e.g., [22, 23]). Hereby, using the Deng-Fan potential [5]

$$U(r) = D_e \left[1 - \frac{e^{\lambda r_e} - 1}{e^{\lambda r} - 1} \right]^2 = A_1 + \frac{A_2}{e^{\alpha r} - 1} + \frac{A_3}{(e^{\alpha r} - 1)^2}, \quad (2)$$

where

$$A_1 = D_e; \quad A_2 = -2D_e(e^{\alpha r_e} - 1); \quad A_3 = D_e(e^{\alpha r_e} - 1)^2,$$

Mustafa [20] has very recently shown (through a quantitative brut-force numerical test) that the factorization recipe

$$\frac{r_e^2}{r^2} = C_0 + \frac{C_1}{e^{\lambda r} - 1} + \frac{C_2}{(e^{\lambda r} - 1)^2}, \quad (3)$$

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of Badawi et al. [21], for the central rotational core $J(J+1)/2\mu r^2$, is a more reliable approximation than that of the improved Greene-Aldrich approximation [22, 23]

$$\frac{1}{r^2} \approx \lambda^2 \left(\frac{1}{12} + \frac{e^{\lambda r}}{(e^{\lambda r} - 1)^2} \right). \quad (4)$$

It has been observed that the larger the rotational quantum number J , the larger are the ro-vibrational energy shifts/deviations, from the numerically predicted ones, for a given vibrational quantum number ν (for more details on this issue see Mustafa [20]). In short, the factorization recipe of Badawi et al. [21] is based on writing the potential and the central rotational term in homogeneous forms and then determine the coefficients C_i 's in terms of the potential parameters.

In the current methodical proposal, we shall use the factorization recipe of Badawi et al.'s [21] and focus on the derivation of an analytical expression for the diatomic molecular ro-vibrational energy levels, that has a sufficiently high accuracy over a relatively broad range of rotational and vibrational quantum numbers. In so doing, we propose a new (to the best of our knowledge, of course) 4-parametric deformed Schiöberg-type [9, 12, 15, 16] potential

$$U(r) = A(B + \tanh_q \alpha r)^2. \quad (5)$$

Where the q -deformation of the usual hyperbolic functions is defined through

$$\tanh_q x = \frac{\sinh_q x}{\cosh_q x}; \quad \sinh_q x = \frac{e^x - qe^{-x}}{2}, \quad \cosh_q x = \frac{e^x + qe^{-x}}{2}. \quad (6)$$

Here, $A > 0, B, q$, and the screening parameter $\alpha > 0$ (which is related to the potential range) are real adjustable parameters to be determined. Nevertheless, a diatomic molecular potential, necessarily and desirably, should satisfy the conditions (usually called Varshni's [6] conditions)

$$\left. \frac{dU(r)}{dr} \right|_{r=r_e} = 0, \quad U(\infty) - U(r_e) = D_e, \quad \text{and} \quad \left. \frac{d^2U(r)}{dr^2} \right|_{r=r_e} = K_e = (2\pi c)^2 \mu \omega_e^2. \quad (7)$$

Where D_e is the dissociation energy, r_e is the equilibrium bond length, c is the speed of light, μ is the reduced mass, and ω_e is the equilibrium harmonic oscillator vibrational frequency. Moreover, the introduction of a fourth condition $U(r_e) = 0$ would only introduce a constant shift (up or down) of the potential curve at the equilibrium bond length, but never violates the three conditions above [11, 12, 14–17]. Therefore, the satisfaction of Varshni's conditions would determine the adjustable parameters A, B , and q of our new deformed Schiöberg potential (5).

On the other hand, the Tietz-Hua oscillator potential [18, 19]

$$U(r) = D_e \left[\frac{1 - e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} \right]^2; \quad b_h = \beta(1 - c_h), \quad \beta = \sqrt{\frac{K_e}{2D_e}}, \quad (8)$$

is known to be one of the very best analytical potentials in the description of molecular dynamics at moderate and high vibrational and rotational quantum numbers. Here, c_h represents an optimization parameter obtained from *ab initio* or Rydberg-Klein-Rees (RKR) intermolecular potentials and β is known as the Morse constant (cf., e.g., [18]). Obviously, in the limit of the optimization parameter $c_h \rightarrow 0$, the Tietz-Hua oscillator potential reduces to the well known Morse oscillator potential [1]. Moreover, when $c_h = e^{-b_h r_e}$ it reduces to Deng-Fan potential (2) (which is shown to be equivalent to the improved Manning-Rosen potential [3, 12, 27]) with $\lambda = b_h$. It is also a straightforward manner to show that the Tietz-Hua oscillator potential is equivalent to the deformed modified Rosen-Morse potential [14, 17, 24, 25].

The organization of current work is in order. In section 2, we use Varshni's conditions (7) to show that our new deformed Schiöberg-type potential (5) and the Tietz-Hua oscillator potential (8) are in fact equivalent. In section 3, we transform our potential (5) into a proper form to be able to use/recycle the supersymmetric quantization recipe of [24] and obtain a closed form solution for the ro-vibrational energy levels. We shall, therefore, only cast the necessary formulae to make the current work self-contained. We discuss our results, in section 4, using 4-diatom molecules $\text{NO}(X^2\Pi_r)$, $\text{O}_2(X^3\Sigma_g^-)$, $\text{O}_2^+(X^2\Pi_g)$, and $\text{N}_2(X^1\Sigma_g^+)$. We compare our results with those of Roy [18], who have used a generalized pseudospectral numerical method (GPS), whenever possible. We give our concluding remarks in section 5.

II. EQUIVALENCE OF THE NEW DEFORMED SCHIÖBERG POTENTIAL AND THE TIETZ-HUA OSCILLATOR

In this section, we shall use Varshni's [6] conditions (7) and show that our new deformed Schiöberg-type potential (5) is equivalent to the Tietz-Hua oscillator potential (8). We start with the application of the first two conditions, in (7), on our potential (5), i. e.,

$$\left. \frac{dU(r)}{dr} \right|_{r=r_e} = 0 \implies B = - \left(\frac{e^{2\alpha r_e} - q}{e^{2\alpha r_e} + q} \right), \quad (9)$$

and

$$U(\infty) - U(r_e) = D_e \implies A = \frac{D_e}{4q^2} (e^{2\alpha r_e} + q)^2. \quad (10)$$

Which when substituted in (5) would yield

$$U(r) = D_e \left[1 - \frac{e^{2\alpha r_e} + q}{e^{2\alpha r} + q} \right]^2. \quad (11)$$

Obviously, the result in (10) implies that the adjustable parameter A is positive whereas the value of B in (9) can be positive or negative, depending on the values of the deformation parameter q . However, applying the third condition, $d^2U(r)/dr^2|_{r=r_e} = K_e$, would imply

$$\beta = \frac{2\alpha e^{2\alpha r_e}}{e^{2\alpha r_e} + q} \implies q = - \left(1 - \frac{b}{\beta} \right) e^{br_e}; \quad b = 2\alpha, \quad \text{and} \quad \beta = \sqrt{\frac{K_e}{2D_e}}. \quad (12)$$

This would immediately suggest that the deformation parameter q may very well be defined as

$$q = -\eta e^{br_e}; \quad \eta = \left(1 - \frac{b}{\beta} \right), \quad (13)$$

where the positivity or negativity of the values of q is determined by the negativity or positivity of the values of the optimization parameter η , respectively. Moreover, it is clear that the deformation parameter q is not an α -independent but rather a deformation function that depends on the spectroscopic parameters b, β , and r_e , i.e., $q \equiv q(b, \beta, r_e) \equiv q(\alpha, \beta, r_e)$. This is the only conclusion one can draw from the third condition of (7).

Under such conditional settings, our new deformed Schiöberg-type potential (5) (hence equivalently (11)) collapses into the Tietz-Hua oscillator potential (8)

$$U(r) = D_e \left[\frac{1 - e^{-b(r-r_e)}}{1 - \eta e^{-b(r-r_e)}} \right]^2, \quad (14)$$

where our $\eta = c_h$ and $b = 2\alpha = b_h$ of Kunc et al.'s [19] and Roy's [18]. The equivalence of our new deformed Schiöberg-type potential (5) and the Tietz-Hua oscillator potential (8) is established, therefore. Yet, the very result of our q -deformation in (13) only documents consistency with the known Tietz-Hua oscillator potential [18, 19], where the spectroscopic parameters of the diatomic molecules (listed in Table 1 below) studied by Kunc et al. [19] and used by Roy [18] are readily known and shall be used here as well.

III. SUPERSYMMETRIC QUANTIZATION AND RO-VIBRATIONAL ENERGY LEVELS

Let us rewrite our new 4-parametric deformed Schiöberg-type potential (5) (which is in fact equivalent to that in (11)) as

$$U(r) = P_1 + \frac{P_2}{e^{br} + q} + \frac{P_3}{(e^{br} + q)^2}; \quad b = 2\alpha, \quad (15)$$

where

$$P_1 = D_e; \quad P_2 = -2D_e (e^{br_e} + q); \quad P_3 = D_e (e^{br_e} + q)^2. \quad (16)$$

At this point, one should notice that Badawi et al. [21] have shown that the Morse-Pekeris, Rosen-Morse, Manning-Rosen, and Tietz potential functions are particular cases of the general expression (15). Obviously, moreover, this potential form (15) represents the first three terms of Eq.(15) in Jia et al.'s [24] work on a 6-parametric exponential-type one-dimensional potential. Where we take $P_4 = P_5 = 0$ of Eq.(15) in [24] and interchange the places of P_2 and P_3 . Hence, the parametric mapping between Jia et al.'s [24] work and our current methodical proposal is made clear. As such, we recycle the supersymmetric quantization recipe of [24] and cast only the necessary formulae to make the current work self-contained.

Next, we incorporate (15) and (16) into (1) and write the effective potential as

$$U_{eff}(r) = \frac{J(J+1)\hbar^2}{2\mu r^2} + U(r) = \tilde{P}_1 + \frac{\tilde{P}_2}{e^{br} + q} + \frac{\tilde{P}_3}{(e^{br} + q)^2}, \quad (17)$$

with

$$\tilde{P}_1 = P_1 + \gamma C_1; \quad \tilde{P}_2 = P_2 + \gamma C_2; \quad \tilde{P}_3 = P_3 + \gamma C_3; \quad \gamma = \frac{J(J+1)\hbar^2}{2\mu r_e^2}. \quad (18)$$

Whilst the values of P_i 's are given in (16), the values of C_i 's are obtained using the factorization recipe of Badawi et al. [21] in the following manner. Let $y = b(r - r_e)$, then with $br = y + u$ and $u = br_e$ one implies that

$$\frac{r_e^2}{r^2} = \frac{1}{(y/u + 1)^2} \quad \text{and} \quad \frac{r_e^2}{r^2} = C_1 + \frac{C_2}{e^{y+u} + q} + \frac{C_3}{(e^{y+u} + q)^2}. \quad (19)$$

Retaining the first three terms of the Taylor's expansion near the equilibrium internuclear distance $y \rightarrow 0$ (i.e., $r \rightarrow r_e$) of both expressions in (19) and equating coefficients of same power of y , one obtains (with $q = -\eta e^{br_e} = -\eta e^u$)

$$C_1 = 1 - \left(\frac{1-\eta}{u}\right)^2 \left[\frac{4u}{1-\eta} - (3+u)\right], \quad (20)$$

$$C_2 = 2e^u(1-\eta) \left[3\left(\frac{1-\eta}{u}\right) - (3+u)\left(\frac{1-\eta}{u}\right)^2\right], \quad (21)$$

$$C_3 = \frac{e^{2u}}{u^2}(1-\eta)^4 \left[(3+u) - \frac{2u}{1-\eta}\right]. \quad (22)$$

Under such potential parametric settings, we may now use the supersymmetric quantum recipe used by Jia et al.[24] and follow, step-by-step, their procedure for our Schrödinger equation in (5), along with the effective potential in (17). Namely, one should set their $P_4 = P_5 = 0$ and their P_1 , P_3 , and P_2 are our current \tilde{P}_1 , \tilde{P}_2 , and \tilde{P}_3 , respectively. Hereby, we only cast the necessary formulae where our superpotential would read

$$\tilde{W}(r) = -\frac{\hbar}{\sqrt{2\mu}} \left(\tilde{Q}_1 + \frac{\tilde{Q}_2}{e^{br} + q} \right), \quad (23)$$

and the one-dimensional ground-state like wave function is given by

$$\psi(r) = N \exp \left(-\frac{\sqrt{2\mu}}{\hbar} \int \tilde{W}(r) dr \right). \quad (24)$$

Which, when substituted in (1) along with (17), would result in

$$\tilde{Q}_2^2 + bq\tilde{Q}_2 = \frac{2\mu}{\hbar^2}\tilde{P}_3 \implies \tilde{Q}_2 = -\frac{bq}{2} \pm \sqrt{\left(\frac{bq}{2}\right)^2 + \frac{2\mu}{\hbar^2}\tilde{P}_3} \quad (25)$$

$$2\tilde{Q}_1\tilde{Q}_2 - b\tilde{Q}_2 = \frac{2\mu}{\hbar^2}\tilde{P}_2 \implies \tilde{Q}_1 = \alpha + \frac{\mu\tilde{P}_2}{\hbar^2\tilde{Q}_2} = \frac{1}{2q\tilde{Q}_2} \left[\frac{2\mu}{\hbar^2} (q\tilde{P}_2 + \tilde{P}_3) - \tilde{Q}_2^2 \right], \quad (26)$$

and

$$\tilde{Q}_1^2 = \frac{2\mu}{\hbar^2} (\tilde{P}_1 - E_0) \implies E_0 = \tilde{P}_1 - \frac{\hbar^2}{2\mu} \left(\frac{1}{2q\tilde{Q}_2} \left[\frac{2\mu}{\hbar^2} (q\tilde{P}_2 + \tilde{P}_3) - \tilde{Q}_2^2 \right] \right)^2. \quad (27)$$

Hence, the wave function reads

$$\psi(r) = N e^{\tilde{Q}_1 r} \left(\frac{e^{br}}{e^{br} + q} \right)^{\tilde{Q}_2/bq} \quad (28)$$

and the corresponding ro-vibrational energy levels (with $b = 2\alpha$) are

$$E_{\nu,J} = \tilde{P}_1 - \frac{\hbar^2 b^2}{2\mu} \left[\frac{\frac{2\mu}{\hbar^2 q^2 b^2} (\tilde{P}_3 + q\tilde{P}_2)}{-1 - 2\nu \pm \sqrt{1 + \frac{8\mu}{\hbar^2 q^2 b^2} \tilde{P}_3}} - \frac{(-1 - 2\nu \pm \sqrt{1 + \frac{8\mu}{\hbar^2 q^2 b^2} \tilde{P}_3})}{4} \right]^2, \quad (29)$$

The positive and negative sings (\pm), however, correspond to positive and negative values of q , respectively. That is, one takes the positive sing for $q > 0$ and the negative sign for $q < 0$. This would, in turn, ensure that the wavefunction (28) vanishes as $r \rightarrow \infty$ and becomes finite as $r \rightarrow 0$. For more details on this issue the reader may refer to Jia et al. [24].

IV. RESULTS AND DISCUSSION

The spectroscopic parameters for 4-diatomic molecules $\text{NO}(X^2\Pi_r)$, $\text{O}_2(X^3\Sigma_g^-)$, $\text{O}_2^+(X^2\Pi_g)$ and $\text{N}_2(X^1\Sigma_g^+)$ as reported by Kunc et al. [19] are summarized in table 1. We now use our result in (29) and calculate the ro-vibrational energy levels listed in table 2 for $\text{NO}(X^2\Pi_r)$, $\text{O}_2(X^3\Sigma_g^-)$, $\text{O}_2^+(X^2\Pi_g)$ molecules, and the vibrational energies for the $\text{N}_2(X^1\Sigma_g^+)$ molecule in table 3. For each of the given diatomic molecules above we have tested the sign of q and accordingly used the proper sign of the square root in (29).

In table 2, we compare our results with those of Roy [18], who have used a GPS numerical method. Roy's results compared excellently with the results of the Nikiforov-Uvarov formalism of Hamzavi et al. [28]. Moreover, in the conversion of the (eV)-units used by Roy [18] into (cm^{-1})-units, we have used the relation

$$E_{\nu,J}(\text{cm}^{-1}) = D_e(\text{cm}^{-1}) + \frac{\text{Roy's}(eV)}{1.23941188 \times 10^{-4} (eV/\text{cm}^{-1})}.$$

It is obvious that our results obtained from (29) are in excellent agreement with those from the GPS numerical method [18] (hence, with the results of the Nikiforov-Uvarov formalism of Hamzavi et al. [28]), whenever available, of course. Yet, in the search for any connection between the accuracy of our results reported in table 2 and the potential parameters listed in table 1, we observe a general trend that the heavier/larger the reduced mass the more accurate our result are compared to GPS ones. This is very much related to the semiclassical limit nature (similar recipes were used early on, like the known large- ℓ expansion technique, cf. e.g., [29–31]) of the Taylor's expansion near the equilibrium internuclear distance, $r \rightarrow r_e$, used in the factorization recipe (19) of Badawi et al. [21]. It is also obvious that the larger the reduced mass, in the central core term $J(J+1)/2\mu r^2$, the less the effect of the rotational quantum number J . The factorization recipe (19) of Badawi et al. [21] is indeed an excellent approximation for the ro-vibrational energy levels.

Furthermore, the authors of [14, 17] have used the common potential (11) (i.e., their Eq.(11) in both [14, 17]) as an equivalent form for their deformed modified Rosen-Morse potential. Therefore, the introduction of table 3 is unavoidably in the process. In this table we compare our results with those reported by Lino da Silva et al. [26] (who have used the RKR method to construct the potential curve of the $\text{N}_2(X^1\Sigma_g^+)$) along with the results reported by Sun et al. [17] and those of Morse potential (i.e., for $\eta = c_h \rightarrow 0$). The comparison between our results and those of Lino da Silva et al. [26] shows that the accuracy is still high (i.e., the accuracy is $\sim 99.1\%$ and is better than that from the Morse, especially for large vibrational quantum numbers ν). However, when we compare our results with those of Sun et al. [17], we observe small discrepancies. These discrepancies are very much related to the improper mathematical argument used by Sun et al. [17] (more details on this issue are discussed in the Appendix below). Moreover, it is a straightforward manner to show that our energy expression (29) is in exact accord with that of Eq.(14) of Sun et al. [17] for the case $J = 0$ they have considered.

V. CONCLUDING REMARKS

In this work, we have introduced a new (to the best of our knowledge) deformed Schiöberg-type potential (5). We have shown that upon the application of Varshni's [6] conditions (7), our deformed potential (5) collapses into

a general/common form (11) shared by a number of well known diatomic potential models. For example, for the Tietz-Hua oscillator potential $q = -\eta e^{br_e}$, $\eta = c_h$, and $2\alpha = b = b_h$ [18, 19], for the Morse oscillator potential [1] $\eta \rightarrow 0$ (i.e., the deformation parameter $q \rightarrow 0$), for the Deng-Fan potential (2) and the improved Manning-Rosen potential [3, 12, 27] $q = -1$ (i.e., $\eta = e^{-br_e}$), etc.

To find a highly accurate (over a wide range of vibrational and rotational quantum numbers) analytical expression for the ro-vibrational energy levels, we have adopted/favoured Badawi et al.'s [21] factorization recipe (to deal with the central rotational core $J(J+1)/2\mu r^2$) and recycled the supersymmetric quantization approach used by Jia et al. [24] for a 6-parametric exponential potential model. Our strategy was inspired by Badawi et al.'s [21] work on writing the potential and the central rotational term in homogeneous forms (i.e., (17) and (19)) and then determine the coefficients C_i 's in terms of the potential parameters to work out an analytical expression (29) for the ro-vibrational energy levels. For the 3-diatomic molecules $\text{NO}(X^2\Pi_r)$, $\text{O}_2(X^3\Sigma_g^-)$, and $\text{O}_2^+(X^2\Pi_g)$ we have used, our results turned out to be highly accurate compared with the numerically predicted ones of Roy [18], who have used a generalized pseudospectral method (GPS) (documented in table 2).

VI. APPENDIX: IMPROPER DETERMINATION OF THE SPECTROSCOPIC PARAMETER α

For the sake of mathematical correctness and scientific honesty, it is deemed unavoidable to introduce table 3 and to pinpoint the mathematical mismanagement in the determination of the spectroscopic parameter α committed by the authors of [14, 17].

In their attempt to determine the spectroscopic parameter α , the authors of [14, 17] have, mathematical wise, mishandled equation (12). They have considered that the deformation parameter q is α -independent and used α values in table 1 to obtain q in (12) (as documented in their q values listed in their table 1 of [14] and used again in [17]). That is, they admit that $q = -\eta e^{br_e} = -c_h e^{br_e}$; $\alpha = b/2$ as given by (12) but again they have used the very same values of α in table 1 to find $\alpha = \alpha_{DMRM}$ (below). This is an odd and/or improper mathematical treatment. Yet, their result (as documented in their Eq.(23) of [17] and Eq.(26) of [14])

$$\alpha_{DMRM} = \frac{1}{2}\beta + \frac{1}{2r_e}W\left(r_e q \beta e^{-r_e \beta/2}\right) ; \quad \beta = \sqrt{\frac{K_e}{2D_e}},$$

should be corrected into

$$\alpha_{DMRM} = \frac{1}{2}\beta + \frac{1}{2r_e}W\left(r_e q \beta e^{-r_e \beta}\right),$$

where W is the Lambert function. However, their approach would remain improper.

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Table 1:

| Molecule | η | $\mu/10^{-23} (g)$ | $\alpha (\text{\AA}^{-1})$ | $r_e (\text{\AA})$ | $\beta (\text{\AA}^{-1})$ | $D_e (cm^{-1})$ | $\omega_e (cm^{-1})$ |
|--------------------------------------------|-----------|--------------------|----------------------------|--------------------|---------------------------|-----------------|----------------------|
| NO ($X^2\Pi_r$) | -0.029477 | 1.249 | 1.357795 | 1.151 | 2.7534 | 53341 | 1904.2 |
| O ₂ ($X^3\Sigma_g^-$) | 0.027262 | 1.377 | 1.295515 | 1.207 | 2.6636 | 42041 | 1580.2 |
| O ₂ ⁺ ($X^2\Pi_g$) | -0.019445 | 1.377 | 1.434935 | 1.116 | 2.8151 | 54688 | 1904.8 |
| N ₂ ($X^1\Sigma_g^+$) | -0.032325 | 1.171 | 1.392925 | 1.097 | 2.6986 | 79885 | 2358.6 |

Table 2:

| | | NO ($X^2\Pi_r$) | | O ₂ ($X^3\Sigma_g^-$) | | O ₂ ⁺ ($X^2\Pi_g$) | |
|-------|-----|-------------------|-----------|------------------------------------|----------|--------------------------------------------|-----------|
| ν | J | GPS [18] | Eq.(29) | GPS [18] | Eq.(29) | GPS [18] | Eq.(29) |
| 0 | 0 | 947.759 | 947.756 | 774.984 | 775.089 | 934.601 | 934.614 |
| | 1 | 951.123 | 951.121 | 777.848 | 777.863 | 937.848 | 937.862 |
| | 2 | 957.849 | 957.847 | 783.394 | 783.410 | 944.341 | 944.353 |
| | 3 | | 967.937 | | 791.731 | | 954.094 |
| | 4 | | 981.390 | | 802.823 | | 967.079 |
| | 5 | | 998.205 | | 816.688 | | 983.310 |
| | 10 | 1132.686 | 1132.686 | 927.562 | 927.578 | 1113.112 | 1113.127 |
| | 15 | 1351.069 | 1351.072 | 1107.634 | 1107.654 | 1323.924 | 1323.940 |
| | 20 | 1653.146 | 1653.153 | 1356.714 | 1356.739 | 1615.541 | 1615.563 |
| 3 | 0 | 6453.267 | 6453.239 | 5269.581 | 5269.672 | 6376.545 | 6376.615 |
| | 1 | 6456.510 | 6456.484 | 5272.250 | 5272.343 | 6379.684 | 6379.756 |
| | 2 | 6462.995 | 6462.971 | 5277.588 | 5277.684 | 6385.962 | 6386.035 |
| | 3 | | 6472.703 | | 5285.694 | | 6395.455 |
| | 4 | | 6485.677 | | 5296.374 | | 6408.015 |
| | 5 | | 6501.894 | | 5309.722 | | 6423.713 |
| | 10 | 6631.552 | 6631.592 | 5416.325 | 5416.479 | 6549.135 | 6549.270 |
| | 15 | 6842.080 | 6842.207 | 5589.607 | 5589.837 | 6752.948 | 6753.159 |
| | 20 | 7133.275 | 7133.526 | 5829.279 | 5829.619 | 7034.867 | 7035.194 |
| 5 | 0 | 9951.736 | 9951.693 | 8118.378 | 8118.516 | 9845.984 | 9846.089 |
| | 1 | 9954.898 | 9954.857 | 8120.977 | 8121.118 | 9849.051 | 9849.159 |
| | 2 | 9961.220 | 9961.188 | 8126.175 | 8126.321 | 9855.183 | 9855.296 |
| | 3 | | 9970.679 | | 8134.126 | | 9864.503 |
| | 4 | | 9983.3351 | | 8144.530 | | 9876.778 |
| | 5 | | 9999.155 | | 8157.535 | | 9892.120 |
| | 10 | 10125.542 | 10125.669 | 8261.257 | 8261.546 | 10014.566 | 10014.830 |
| | 15 | 10330.775 | 10331.112 | 8429.966 | 8430.441 | 10213.639 | 10214.091 |
| | 20 | 10614.632 | 10615.269 | 8663.303 | 8664.046 | 10488.989 | 10489.719 |

Table 3:

| ν | RKR [26] | DMRM [17] | Eq.(29) | Morse [17] |
|-------|-----------|-----------|-----------|------------|
| 0 | 1184.4539 | 1174.9971 | 1174.9270 | 1174.9477 |
| 1 | 3526.3576 | 3499.8409 | 3499.7430 | 3498.7289 |
| 2 | 5833.4516 | 5790.8755 | 5790.7601 | 5787.6913 |
| 3 | 8107.0460 | 8048.0809 | 8047.9316 | 8041.8351 |
| 4 | 10348.312 | 10271.387 | 10271.210 | 10261.160 |
| 5 | 12558.287 | 12460.752 | 12460.549 | 12445.666 |
| 6 | 14737.876 | 14616.138 | 14615.901 | 14595.353 |
| 7 | 16887.859 | 16737.473 | 16737.218 | 16710.222 |
| 8 | 19008.895 | 18824.747 | 18824.454 | 18790.272 |
| 9 | 21101.519 | 20877.869 | 20877.559 | 20835.503 |

Tables captions:

Table 1: Spectroscopic parameters and constants used in this work, quoted from [18].

Table 2: Ro-vibrational energies $E_{\nu,J}$ (in cm^{-1} units) for 3-diatomic molecules with $\nu = 0, 3, 5$ and different value of J . Our results in (29) are compared with those of Roy's [18] (GPS) whenever possible.

Table 3: Vibrational energies $E_{\nu,J}$ (in cm^{-1} units) for N_2 ($X^1\Sigma_g^+$). Our results (29) are compared with those of RKR [26], DMRM [17], and Morse [17].